Alternative Calibration Examination

1/21/2020

623721

Conclusions

- Alternative calibrations are equivalent to or better in quality than CPG calibration when looking at the SPAF metric, MLE metric, and dynamic time series compared to data
- Alternative calibrations can result in different results within long-term projections
- High quality calibrations were achieved both Kow-Constant runs and Kow-Variable runs

Conclusions (2)

- Model parameters varied widely across optimal calibrations, suggesting a unique “best” parameterization does not exist.
- Biotic data averaging techniques have little impact on model calibrations
  - e.g. whether to include fillet data with conversions or whether to include organisms caught near to but not within a reach
  - even when the model was calibrated to these alternative central tendencies, time-series model results looked quite similar

Runs Completed

- CPG Calibration
- Optimize SPAF to Priority Species (SPAF P)
  - with and without holding Kow Constant
- Optimize SPAF for all Species (SPAF A)
  - with and without holding Kow Constant
- Optimize Maximum Likelihood (MLE)
  - with and without holding Kow Constant

- All runs were performed twice using EPA and CPG biotic data management

Runs completed and metrics

Optimizer Goal	Log Kow	Biotic Data Management	Avg. Priority SPAF	Avg SPAF, All Orgs.	Log Likelihood
MLE	Vary	CPG	1.41	3.51	-246.35
MLE	Const	CPG	1.53	3.92	-333.97
SPAF P	Vary	CPG	1.12	5.13	-1182.30
SPAF P	Const	CPG	1.19	5.96	-1199.12
SPAF A	Vary	CPG	1.66	2.32	-381.00
SPAF A	Const	CPG	2.09	2.69	-679.01
N / A	Const	CPG	1.96	4.74	-834.10
MLE	Vary	EPA	1.47	3.20	-315.08
MLE	Const	EPA	1.65	3.35	-355.50
SPAF P	Vary	EPA	1.16	4.99	-605.39
SPAF P	Const	EPA	1.22	5.53	-704.72
SPAF A	Vary	EPA	1.60	2.17	-421.55
SPAF A	Const	EPA	1.99	2.53	-627.56

SPAFs for priority Species

Model produced very low SPAFs for priority species when Kow was varied

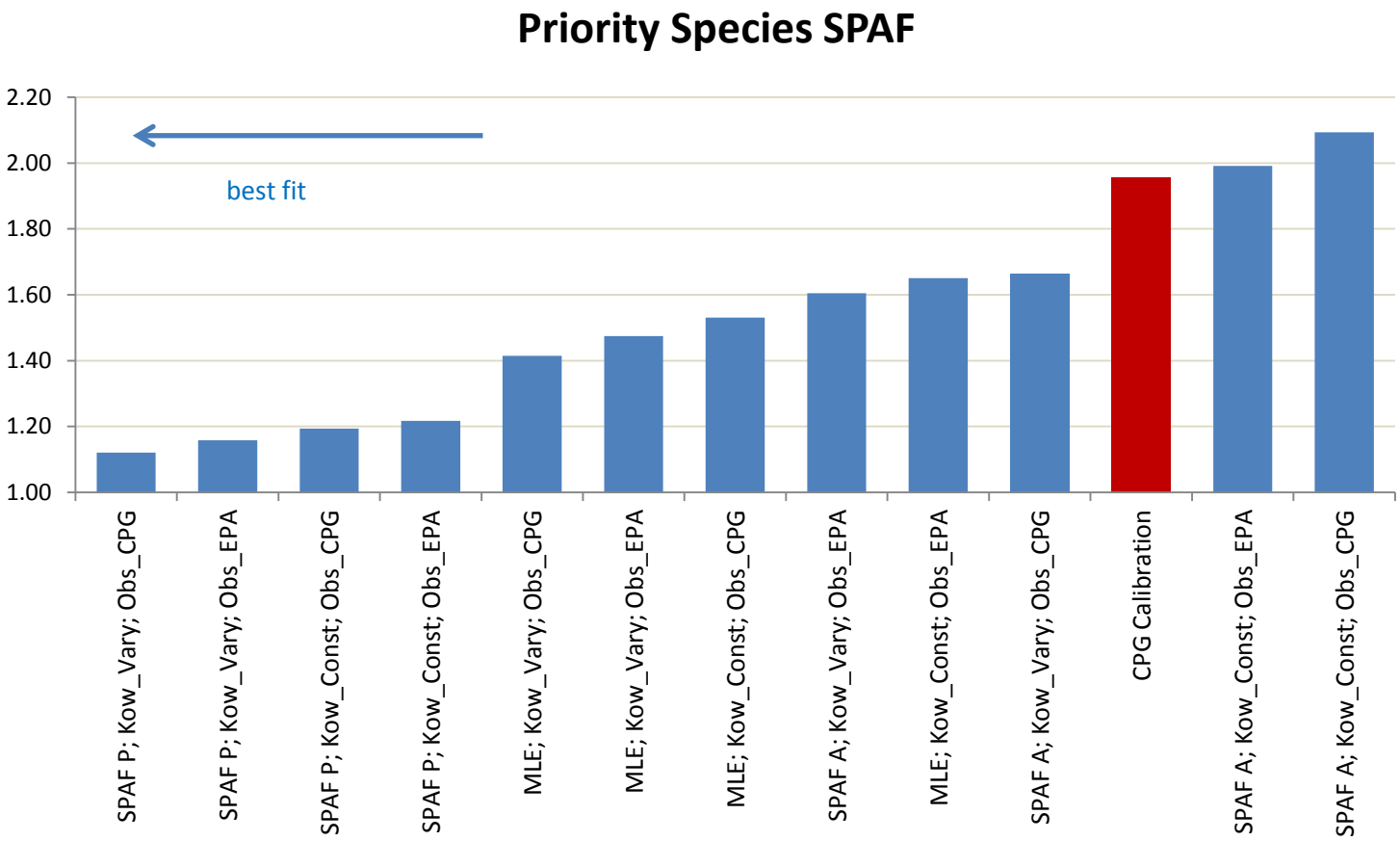
	2378 TCDD			Tetra CB		
	RM 0-6	**RM 6-14.7**	**RM 14.7-Dam**	**RM 0-6**	**RM 6-14.7**	**RM 14.7-Dam**
DEP (Invert)		26.9	17.6		8.6	12.5
FF (Invert)						
DET (Invert)						
C/O (Invert)	31.5			15.1		
Small FF fish		1.1			-1.4	
Small forage fish	-1.8	**-1.0**	-14.9	1.1	**1.0**	1.0
Small American eel	-5.0	**-1.0**	-2.1	-2.1	**-1.0**	1.3
Blue crab	**-1.5**	**1.5**	-15.7	**-1.1**	**1.2**	1.4
Carp		**-1.0**	-3.2		**-1.2**	2.1
Catfish	-5.2	**-1.0**	-42.7	-2.4	**1.2**	1.0
White perch	**-1.2**	**1.3**	-8.2	**-1.1**	**-1.0**	1.6
Large American Eel	-1.2	**-1.0**		-1.7	**-1.0**	
Bass		**1.0**	-2.4		**1.0**	-1.5
Average All	2.6	1.1	12.8	1.6	1.1	1.4
Average Priority	**1.16**			**1.09**		

SPAFs for priority Species – Kow Const.

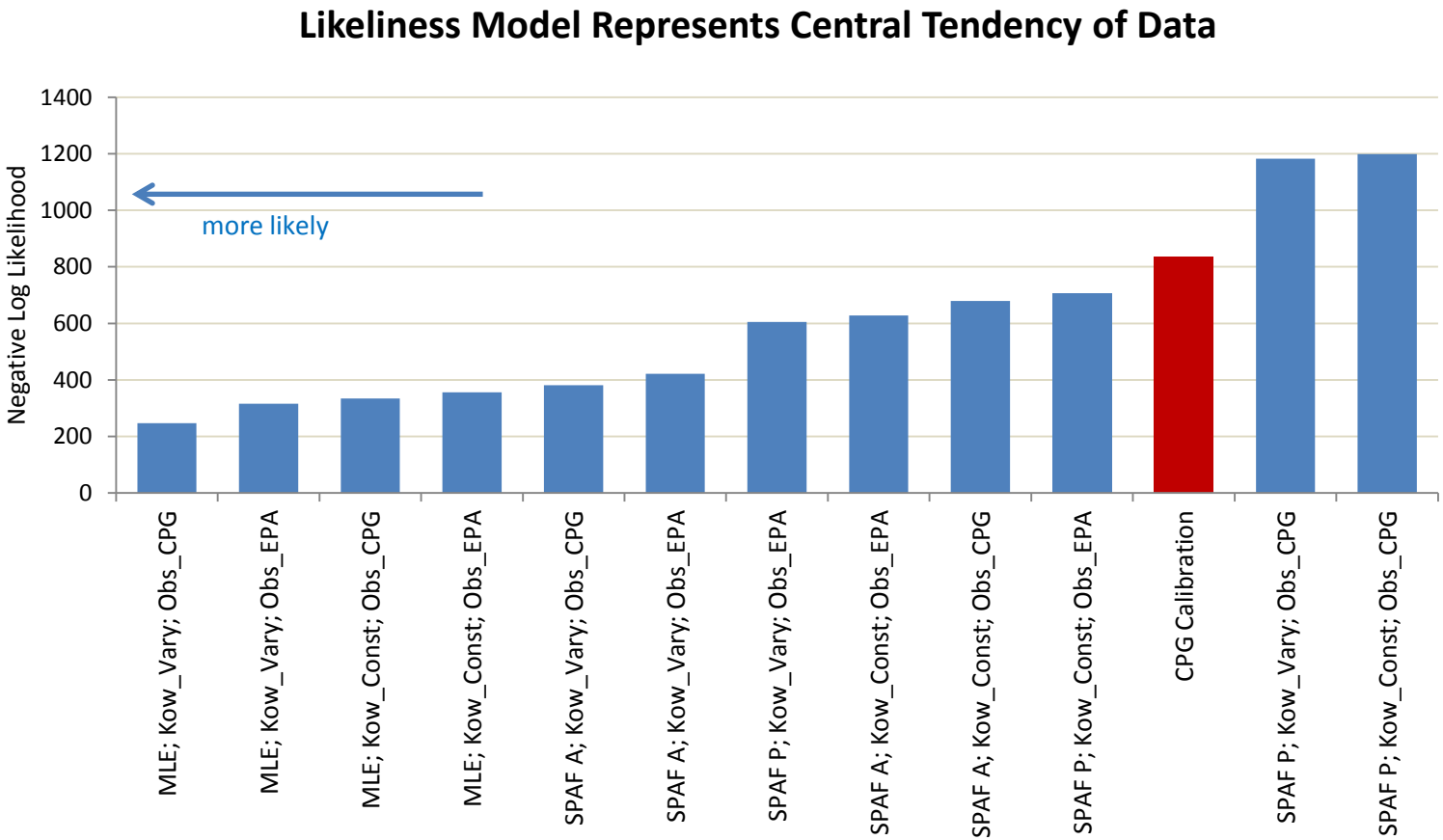
Model also produced low SPAFs for priority species when Kow was constant

	2378 TCDD			Tetra CB		
	RM 0-6	**RM 6-14.7**	**RM 14.7-Dam**	**RM 0-6**	**RM 6-14.7**	**RM 14.7-Dam**
DEP (Invert)		37.3	19.5		8.3	11.6
FF (Invert)						
DET (Invert)						
C/O (Invert)	38.5			13.8		
Small FF fish		1.1			-1.4	
Small forage fish	-2.0	**-1.0**	-19.2	1.0	**1.0**	-1.1
Small American eel	-4.8	**1.0**	-1.9	-2.0	**-1.0**	1.3
Blue crab	**-1.7**	**1.6**	-18.8	**-1.2**	**1.3**	1.3
Carp		**-1.0**	-3.9		**-1.4**	1.6
Catfish	-5.6	**1.0**	-55.2	-2.8	**1.1**	-1.1
White perch	**-1.5**	**1.5**	-9.8	**-1.4**	**-1.1**	1.3
Large American Eel	-1.5	**-1.0**		-1.8	**1.0**	
Bass		**1.0**	-3.2		**-1.1**	-1.7
Average All	2.8	1.1	16.0	1.7	1.2	1.3
Average Priority	**1.22**			**1.16**		

SPAF for Priority Species

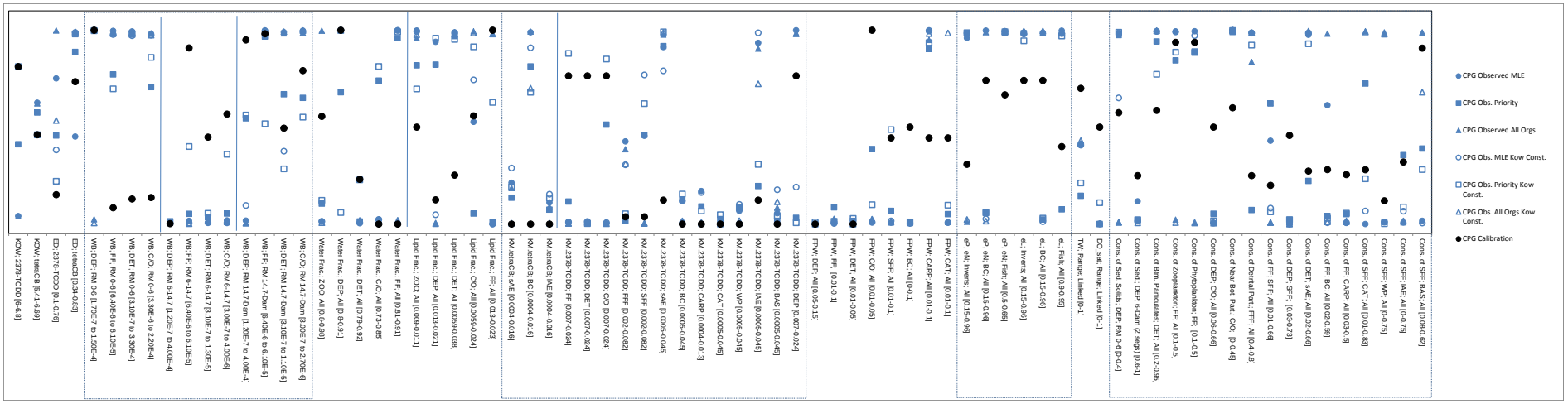


Maximum Likelihood for all Biotic Data



Parameter Results

- all parameters are shown plotted against their uncertainty ranges
  - the five calibrations are “CPG Calibration,” “optimized to MLE,” “optimized to SPAF priority,” and the two optimizations holding Kow Constant. (Used CPG biotic-data central tendencies.)
- a birds eye view suggests significant variation in most parameters
- even in these five “quality” calibrations, parameters can vary quite a bit
- i.e. no unique model calibration



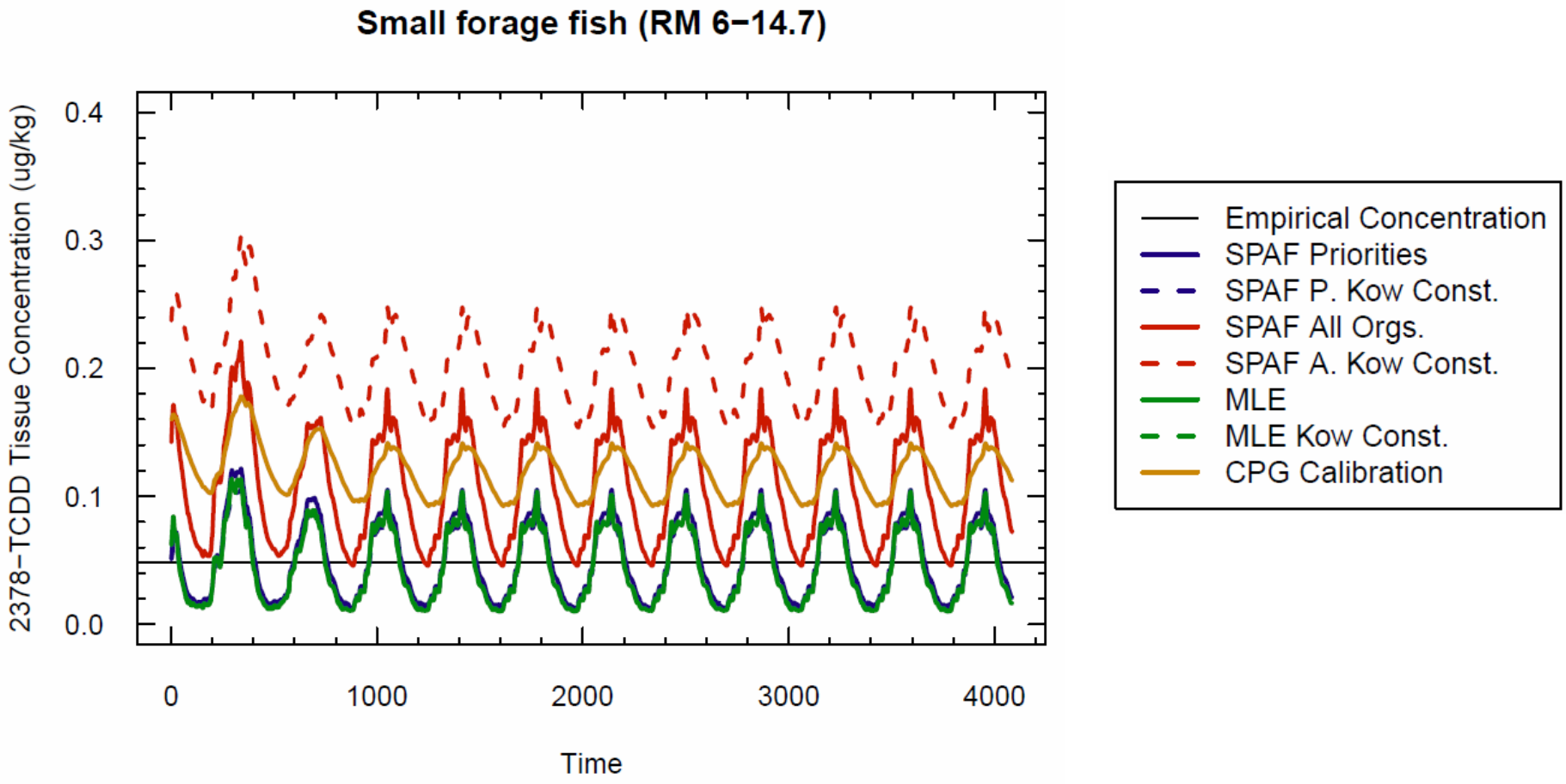
Time Series Results

- Alternative calibrations were tested in the kinetic model
- The original 2007-2010 time series was extended to 2018 by repeating the last year
  - September of 2009-September 2010
    - consistent with 2010 fish collection dates
  - this was done to examine model behavior over a long term run – i.e.
- CPG kinetic-model tests initialized organisms using observed biotic data
  - initializing the model to observed data provides a less robust test of the model calibration
  - in these runs, biota were initialized using steady-state model results

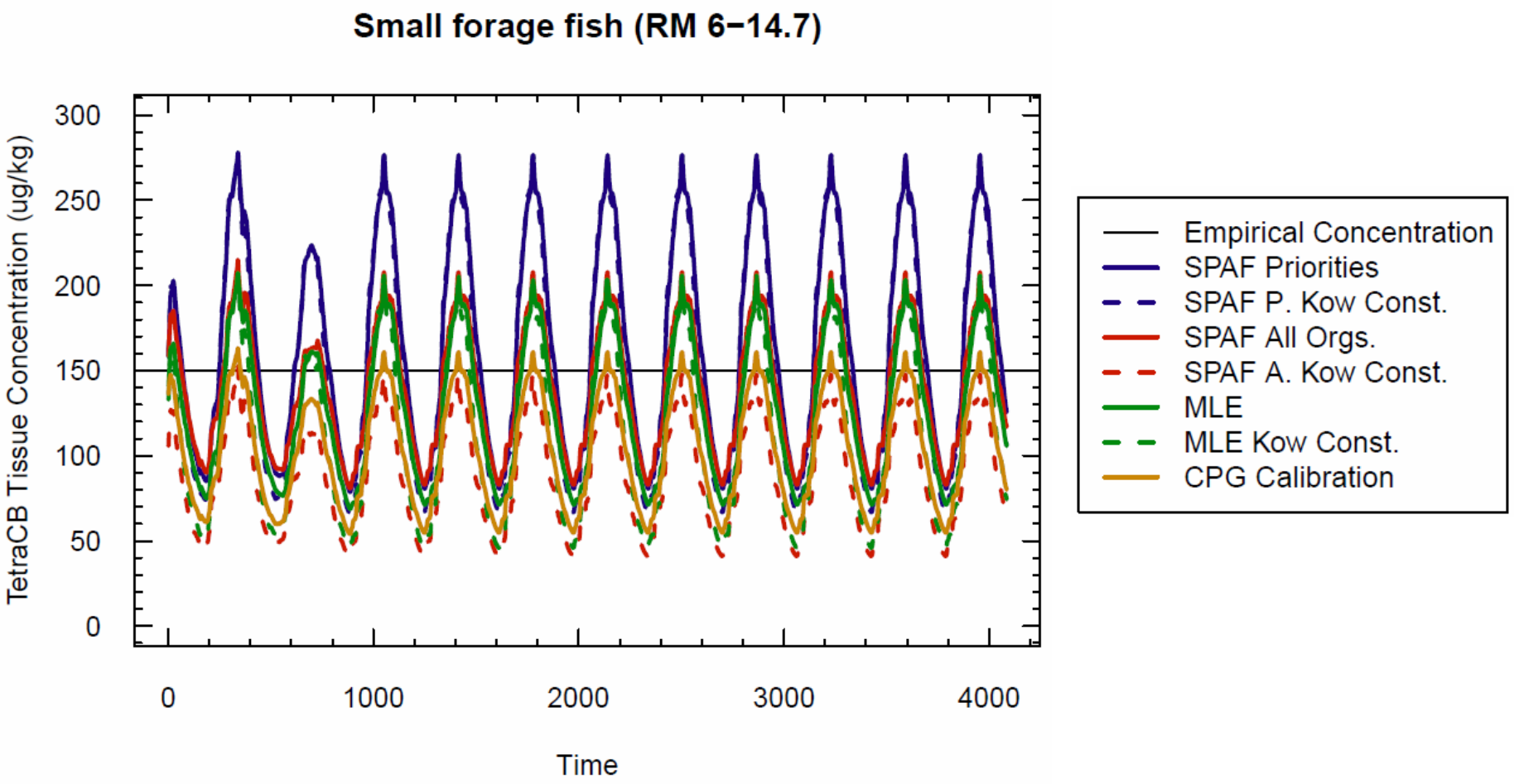
Time Series Conclusions

- Optimized calibrations seem to generally outperform the CPG calibration in the time-series runs
- The optimization goal has a greater impact on model predictions than the choice of whether to vary Kow or not

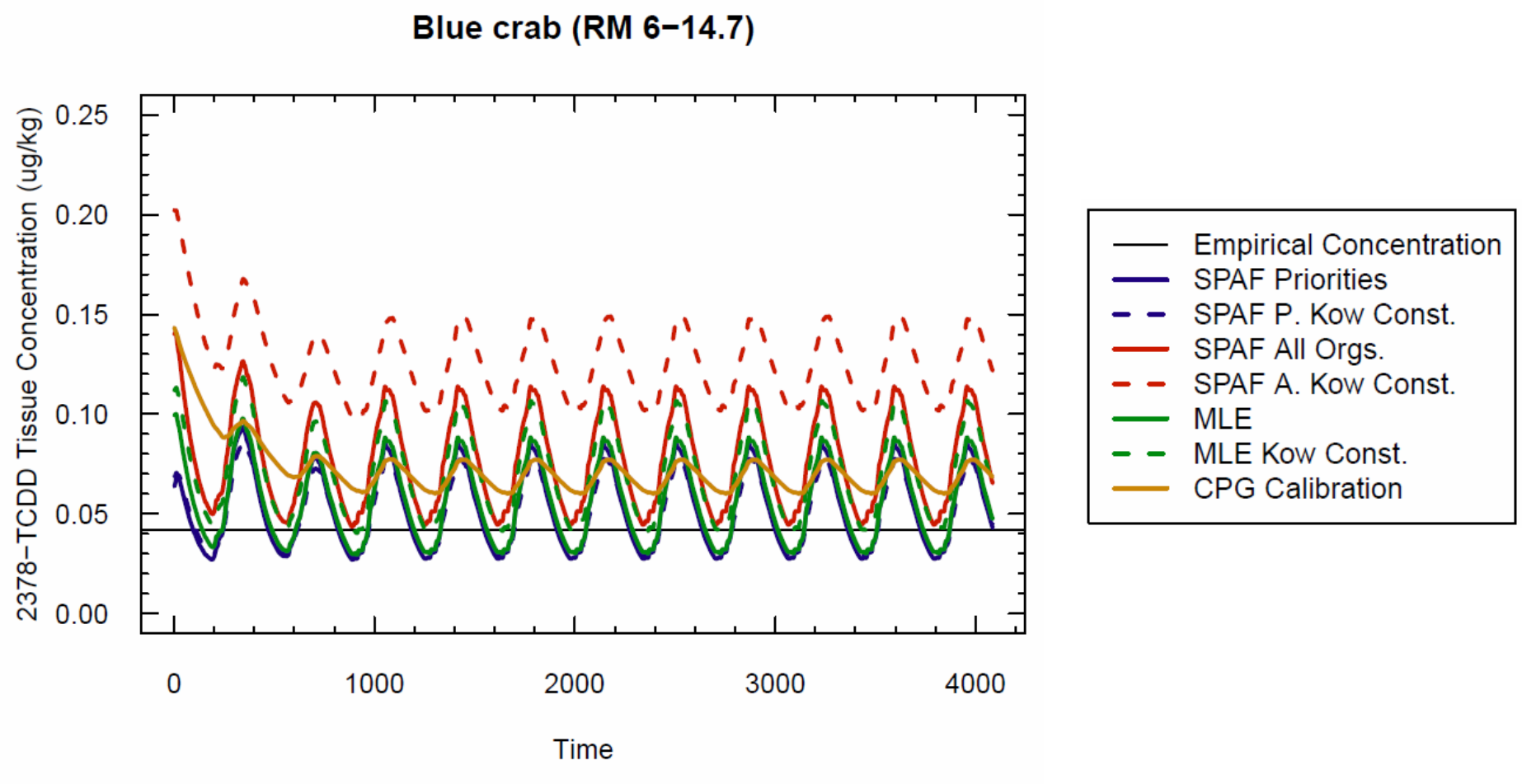
2,3,7,8 TCDD in forage fish



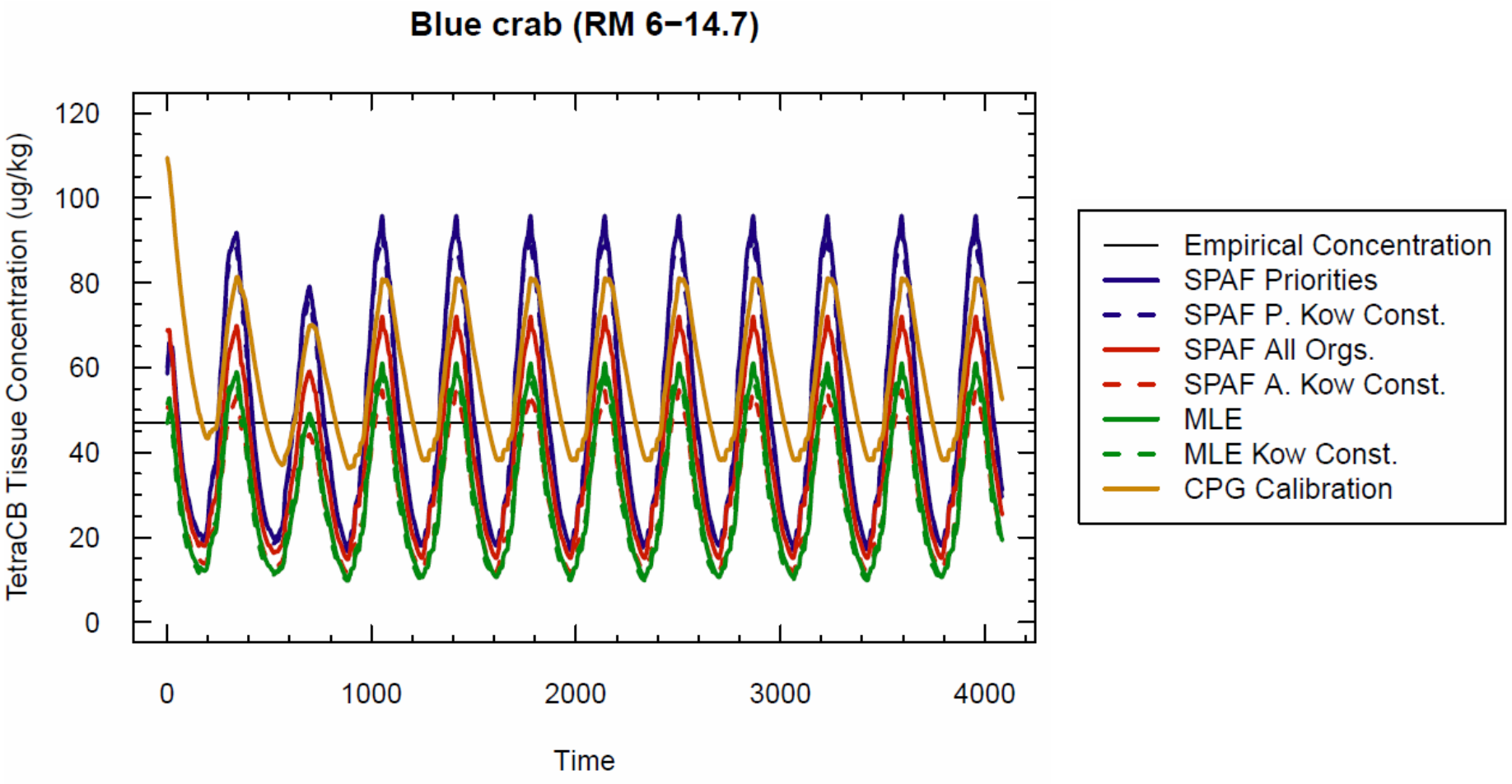
Tetra CB in forage fish



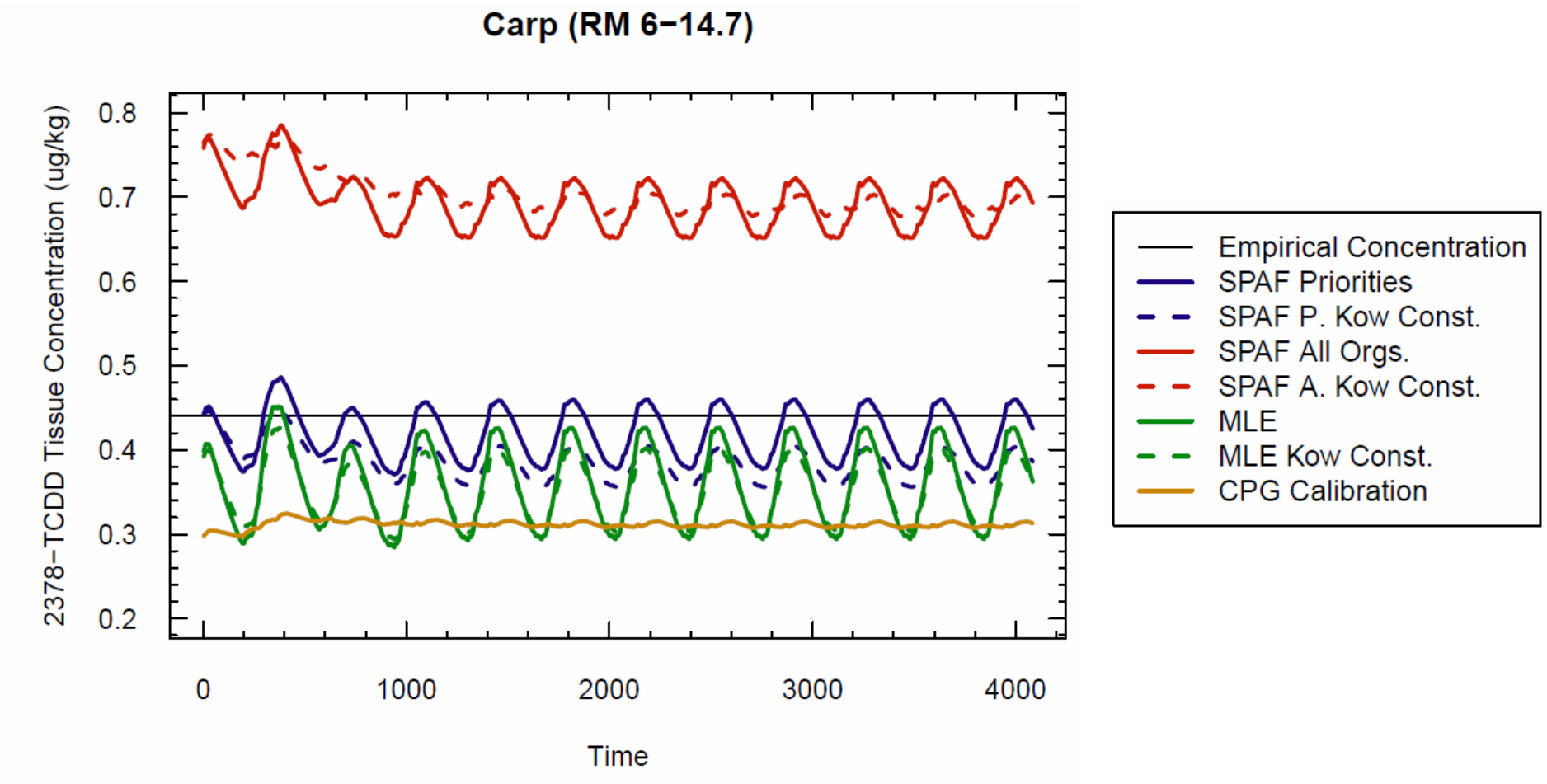
2,3,7,8 TCDD in blue crab



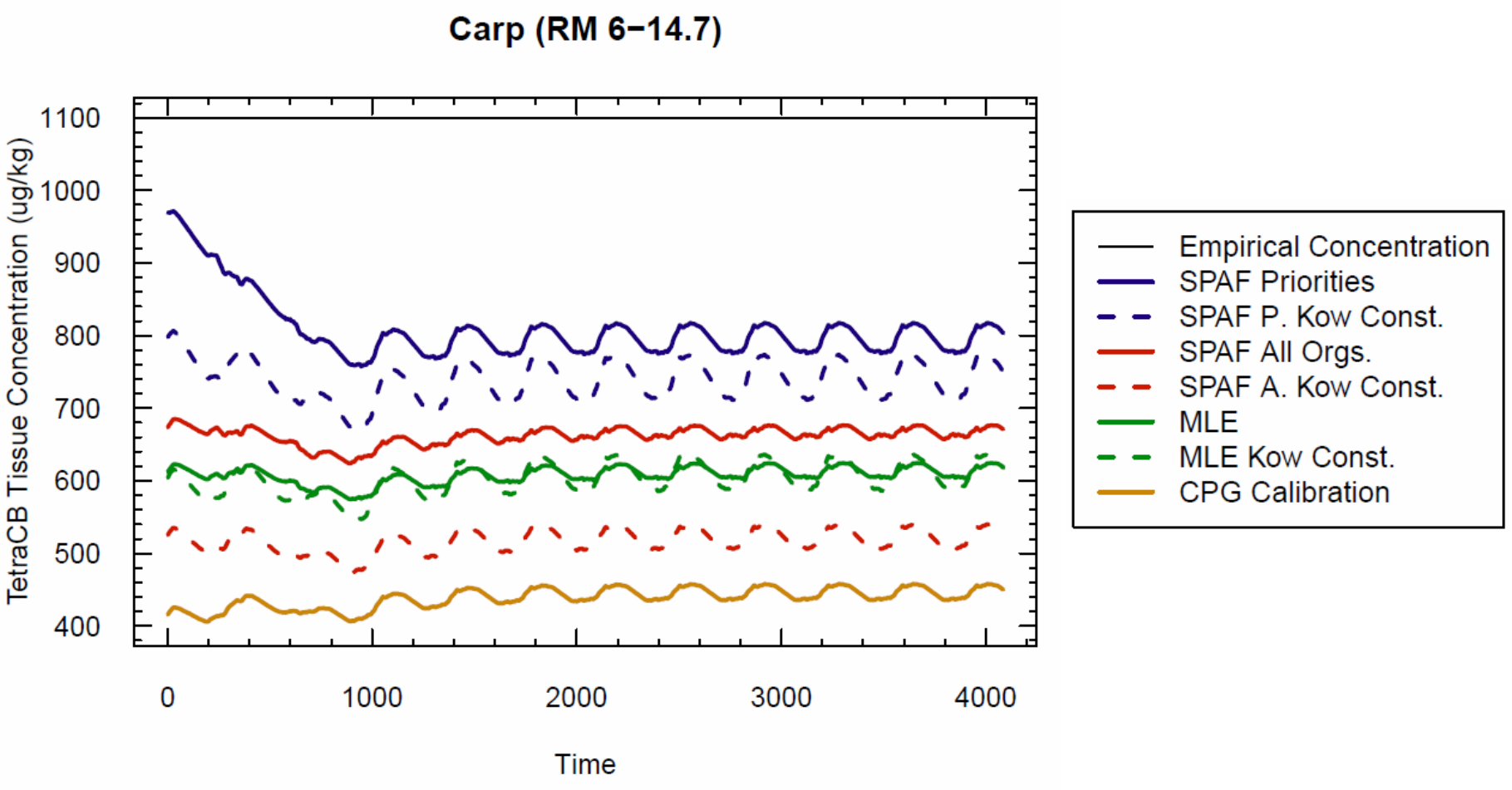
Tetra CB in blue crab



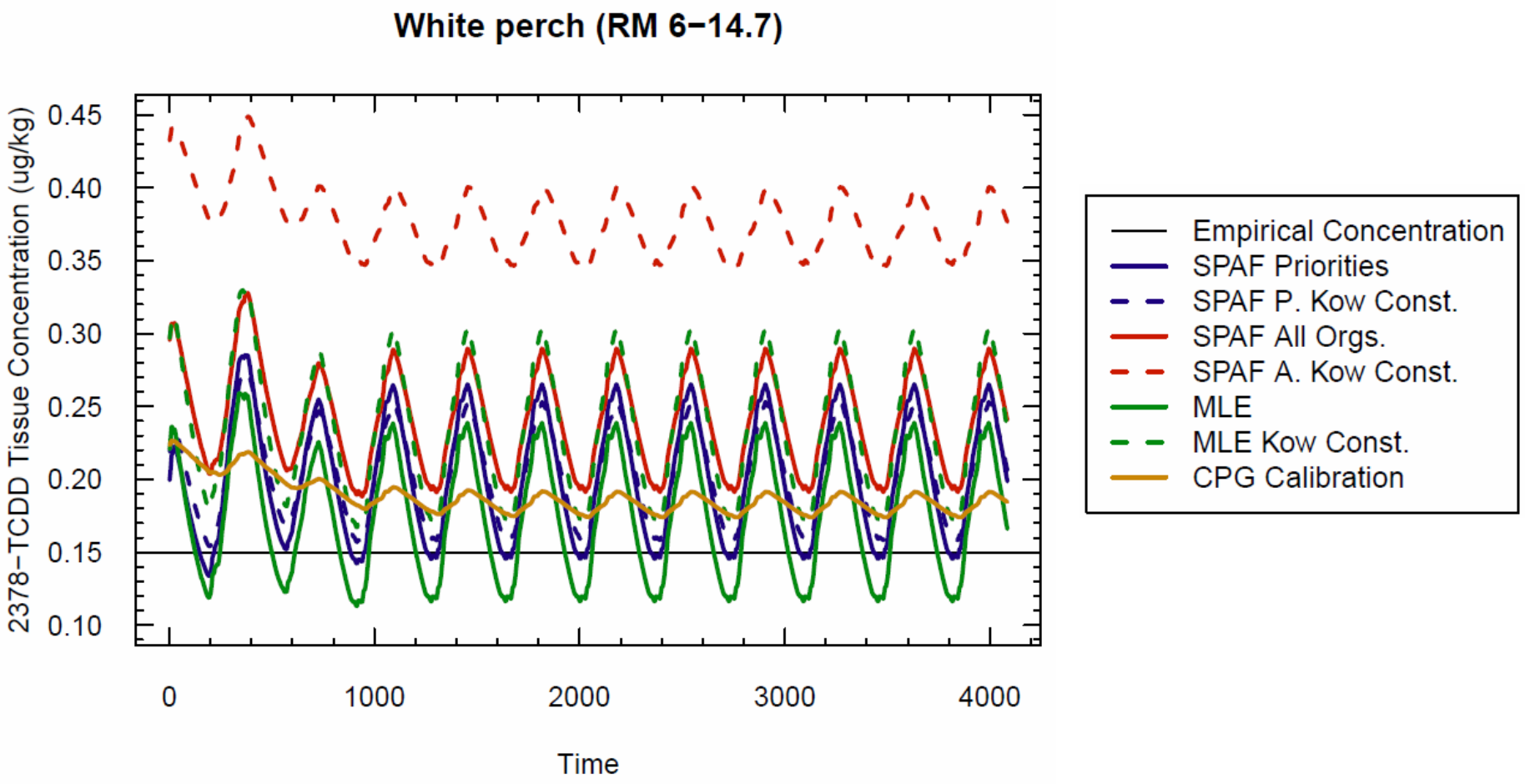
2,3,7,8 TCDD in carp



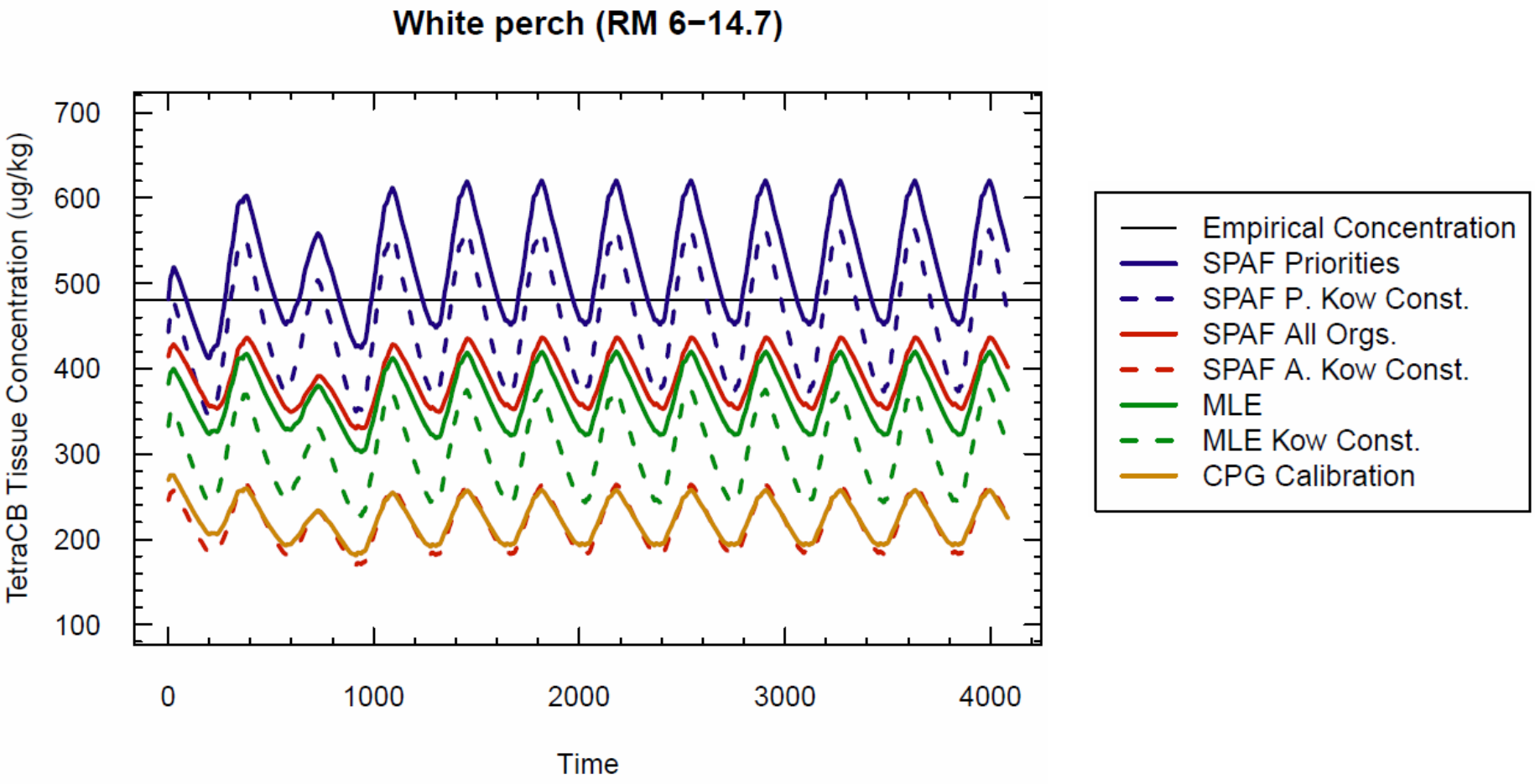
Tetra CB in carp



2,3,7,8 TCDD in white perch



Tetra CB in white perch



Parameter observations

- Kow
  - optimizer prefers lower Kow for 2378 TCDD (6.05 to 6.5)
  - prefers higher Kow for Tetra CB (6.15 to 6.3)
- ED
  - optimizer prefers higher ED for 2378 TCDD (0.25 to 0.75)
  - mixed results on Tetra CB
- Weights
  - invertebrate weights vary by reach
    - this provides a reach-specific “dial” to turn up or down contaminant concentrations
      - Original EPA optimizations did not vary invertebrate weights by reach for this reason
    - in general, in RM 0-6 higher weights are preferred (not DEP)
    - in RM 6-14.7 lower weights are preferred

Parameter observations (cont.)

- Water Fraction and Lipid Fraction
  - no consistent pattern
- Metabolism – varies by organism
  - for Tetra CB, higher KM for blue crab, lower for eel
  - for 2,3,7,8 TCDD Mixed Results
    - higher KMs for forage fish, small and large eels
    - lower KMs for carp, catfish, white perch, blue crab
- Fraction Pore Water
  - generally mixed, except high exposure for carp
- Water Temperature
  - somewhat lower than CPG calibration is optimal

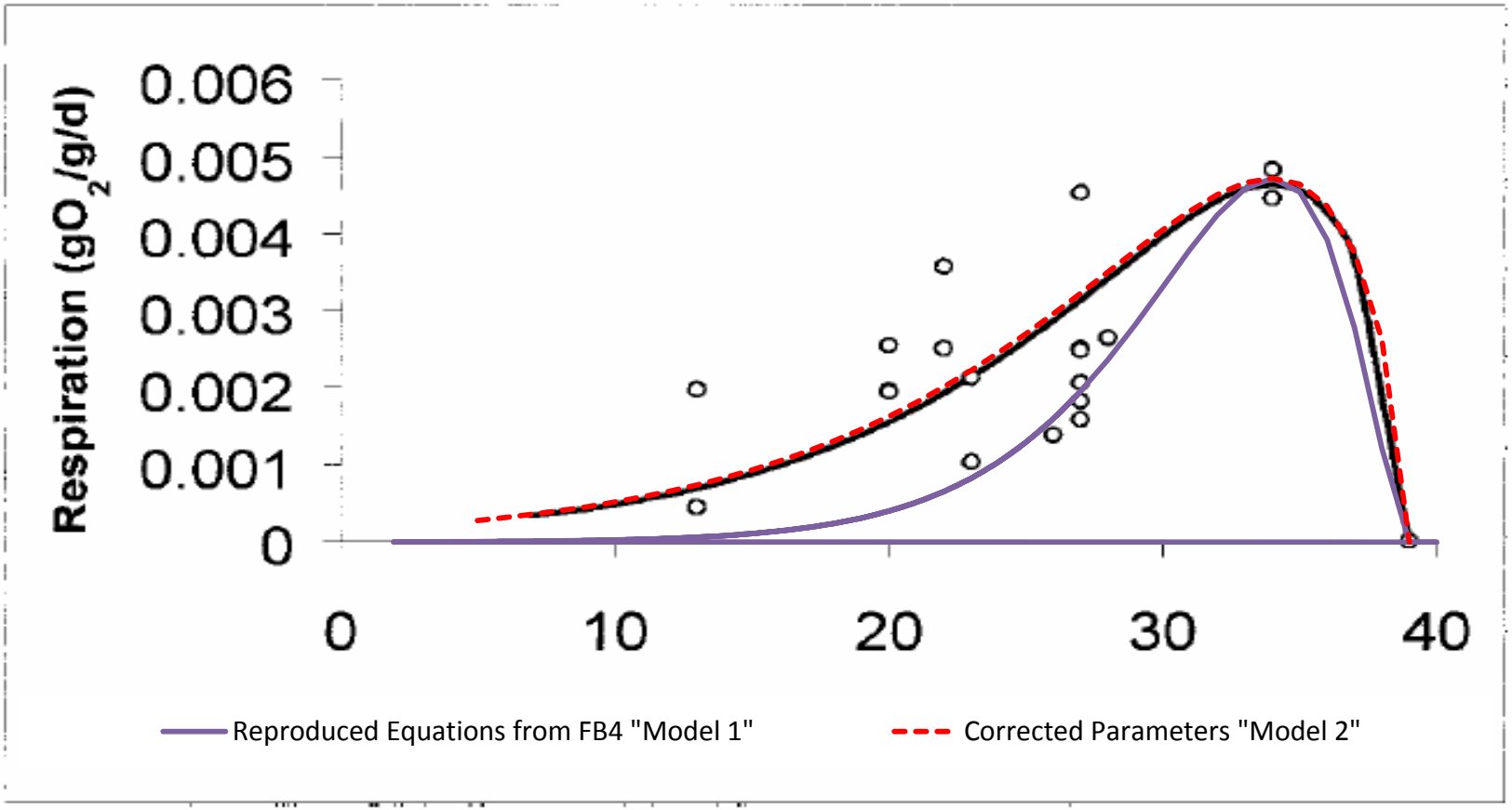
Parameter observations (diet)

- Optimizer results agree that for best calibration:
  - DEP, RM 6-Dam, consumes lower sediment
    - closer to 60% than 100%
  - DET consumes higher bottom particulates
    - closer to 95% than 20%
  - C/O consumes lower DEP
    - closer to 60% than 6%
  - Small Forage Fish consumes lower DEP
    - closer to 3% than 73%
  - Carp consumes lower filter feeder
    - closer to 3% than 50%.

Blue Crab Bioenergetics Update

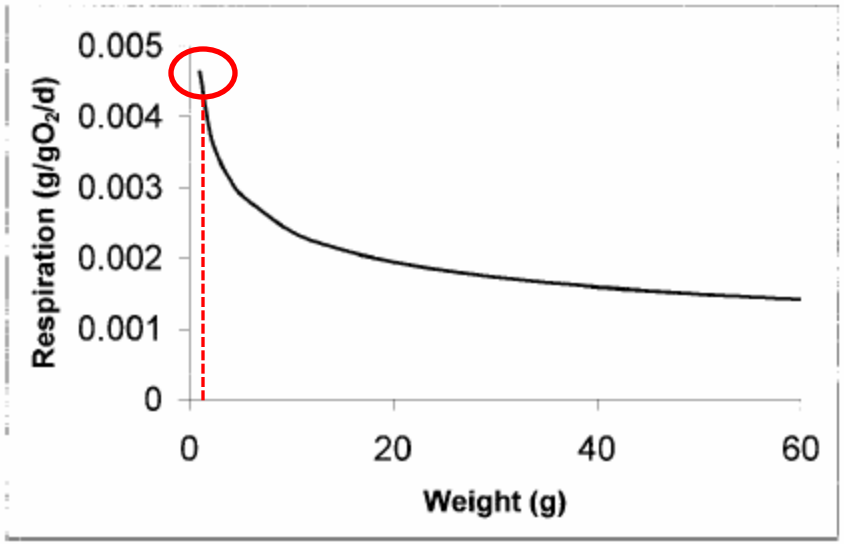
- Parameter error found in literature paper used for blue-crab bioenergetics
  - Brylawski and Miller (2003)
  - Published parameters “Model 1”
- Update was sent in September of 2019
  - Updated parameters “Model 2”
- Further refinements to report here
  - Memo update 1-21-2020
  - Adult blue-crab model -- “Model 3”

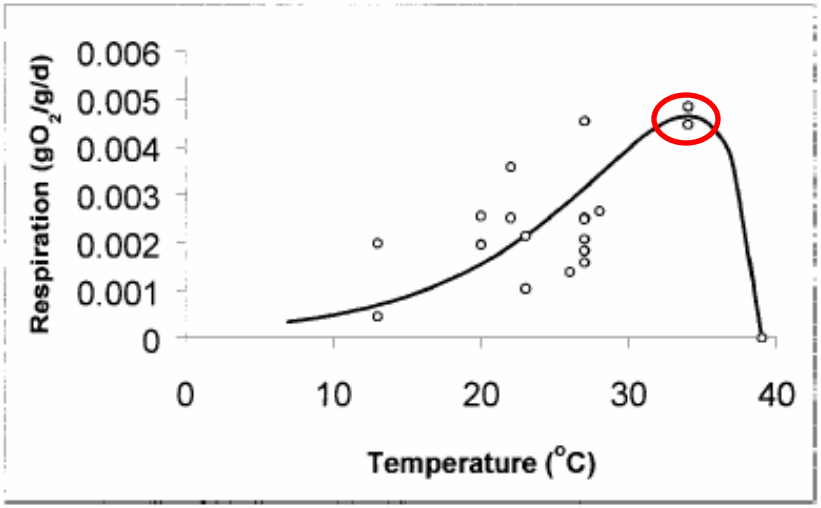
Original parameter error discovered in September 2019



Further refinement

- Comparing Figure 3 and Figure 4, one can see that the model presented in Figure 4 is for a ~1-gram crab

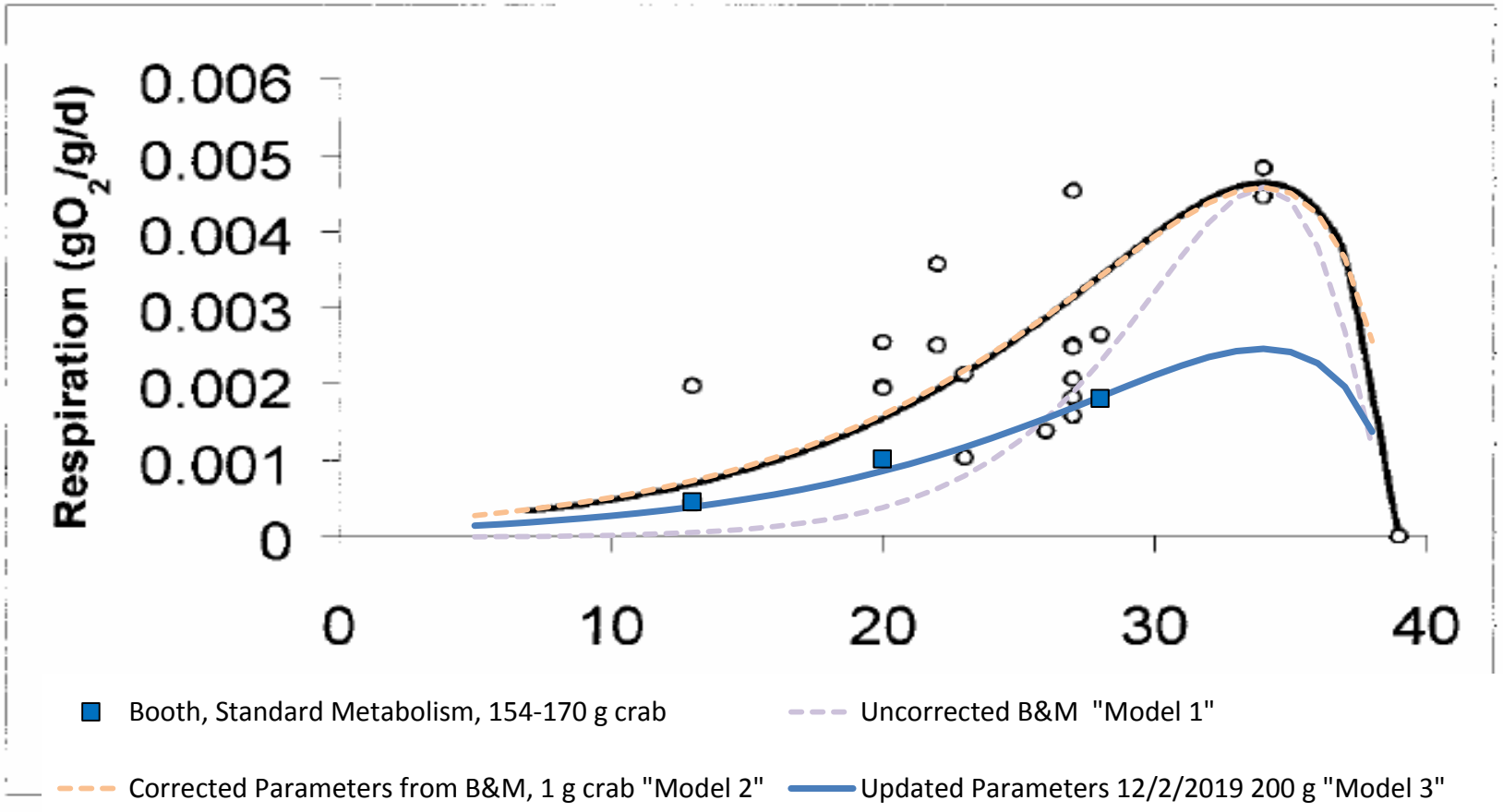




- Need a model for 140-170 g crab

Proposed Updated Model

"Model 3" increases Blue-Crab contaminant predictions by ~20% compared to "Model 1," which is used in CPG calibration



SPAFs for priority Species

The Alt Calibration used “Model 2”

Model produced very low SPAFs for priority species when Kow was varied

	2378 TCDD			Tetra CB		
	RM 0-6	**RM 6-14.7**	**RM 14.7-Dam**	**RM 0-6**	**RM 6-14.7**	**RM 14.7-Dam**
DEP (Invert)		26.9	17.6		8.6	12.5
FF (Invert)						
DET (Invert)						
C/O (Invert)	31.5			15.1		
Small FF fish		1.1			-1.4	
Small forage fish	-1.8	**-1.0**	-14.9	1.1	**1.0**	1.0
Small American eel	-5.0	**-1.0**	-2.1	-2.1	**-1.0**	1.3
Blue crab	**-1.5**	**1.5**	-15.7	**-1.1**	**1.2**	1.4
Carp		**-1.0**	-3.2		**-1.2**	2.1
Catfish	-5.2	**-1.0**	-42.7	-2.4	**1.2**	1.0
White perch	**-1.2**	**1.3**	-8.2	**-1.1**	**-1.0**	1.6
Large American Eel	-1.2	**-1.0**		-1.7	**-1.0**	
Bass		**1.0**	-2.4		**1.0**	-1.5
Average All	2.6	1.1	12.8	1.6	1.1	1.4
Average Priority	**1.16**			**1.09**		

SPAFs for priority Species

(Same parameters but with Blue Crab "Model 3")

Very small differences, blue crab calibration seems improved overall.
Alt Calibration was not significantly affected by using "Model 2" vs "3"

	2378 TCDD			Tetra CB		
	RM 0-6	**RM 6-14.7**	**RM 14.7-Dam**	**RM 0-6**	**RM 6-14.7**	**RM 14.7-Dam**
DEP (Invert)		26.9	17.6		8.6	12.5
FF (Invert)						
DET (Invert)						
C/O (Invert)	31.5			15.1		
Small FF fish		1.1			-1.4	
Small forage fish	-1.8	**-1.0**	-14.9	1.1	**1.0**	1.0
Small American eel	-5.0	**-1.0**	-2.1	-2.1	**-1.0**	1.3
Blue crab	**-1.6**	**1.4**	-17.0	**-1.2**	**1.1**	1.2
Carp		**-1.0**	-3.2		**-1.2**	2.1
Catfish	-5.2	**-1.0**	-42.7	-2.4	**1.2**	1.0
White perch	**-1.2**	**1.3**	-8.2	**-1.1**	**-1.0**	1.6
Large American Eel	-1.2	**-1.0**		-1.7	**-1.0**	
Bass		**1.0**	-2.4		**1.0**	-1.5
Average All	2.7	1.1	12.9	1.6	1.1	1.4
Average Priority	**1.15**			**1.08**		

Use of Alt. Calibration Analysis

- Several options:
  - Use one of the alt. calibration runs as primary calibration– improved SPAFs and other calibration metrics
  - Or -- carry the set of runs forward as alt. calibration, uncert-analysis

- CPG Calibration
  - Fix the kinetic-model initialization problem
    - Do not initialize the model with observed data
  - Fix the blue-crab bioenergetics issue
  - Use some of the parameter observations to improve calibration?